

Entanglement of two delocalised electrons

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(Dated: 20 March 2006)

Several convenient formulae for the entanglement of two indistinguishable delocalised spin- $\frac{1}{2}$ particles are introduced. This generalizes the standard formula for concurrence, valid only in the limit of localised or distinguishable particles. Several illustrative examples are given.

PACS numbers: 03.67.Mn, 03.67.Pp, 73.63.-b

Entanglement is a well-defined quantity for two distinguishable qubits in a nonfactorizable quantum state, where it may be uniquely defined through von Neuman entropy and concurrence [1, 2, 3, 4]. However, amongst the realistic systems of major physical interest, electron-qubits have the potential for a much richer variety of entanglement measure choices due to both their charge and spin degrees of freedom. For example, in lattice fermion models such as the Hubbard dimer, entanglement is sensitive to the interplay between charge hopping and the avoidance of double occupancy due to Hubbard repulsion, which results in an effective Heisenberg interaction between adjacent spins [5]. In systems of identical particles the main challenge is to define an appropriate entanglement measure which adequately deals with multiple occupancy states [6, 7, 8, 9, 10, 11]. In the case of fermions such a measure must also account for the effect of exchange [12] as well as of mutual electron repulsion.

Entangled fermionic qubits can be created with electron-hole pairs in a Fermi sea [13] and in the scattering of two distinguishable particles [14]. A spin-independent scheme for detecting orbital entanglement of two-quasiparticle excitations of a mesoscopic normal-superconductor system was also proposed recently [15].

A consensus regarding the appropriate generalization of entanglement measure which would consider spin and orbital entanglement of electrons on the same footing has not, however, been reached yet. In any realistic solid-state device, spin entanglement is intimately related to the orbital degrees of freedom of the carriers, which cannot be ignored, even in otherwise pure spin entanglement observations. In this paper we introduce spin-entanglement measure formulae valid for real electrons and show how, in general, spin-entanglement depends in an essential way on spatially delocalised orbitals.

For two distinguishable particles A and B , each described with single spin- $\frac{1}{2}$ (or pseudo spin) states $s = \uparrow$ or \downarrow and in a pure state $|\Psi_{AB}\rangle = \sum_{ss'} \alpha_{ss'} |s\rangle_A |s'\rangle_B$ concurrence as a measure of entanglement is given by [2]

$$C = 2|\alpha_{\uparrow\uparrow}\alpha_{\downarrow\downarrow} - \alpha_{\uparrow\downarrow}\alpha_{\downarrow\uparrow}|. \quad (1)$$

Concurrence is related to the density matrix of a pair

of spins [4] and can be expressed in terms of spin-spin correlators $\langle \Psi_{AB} | S_A^\lambda S_B^\mu | \Psi_{AB} \rangle$ and expectation values $\langle \Psi_{AB} | S_{A(B)}^\lambda | \Psi_{AB} \rangle$, where $S_{A(B)}^\lambda$ for $\lambda = x, y, z$ are spin operators corresponding to spin A or B , respectively. This approach has proved to be efficient in the analysis of entanglement in various spin-chain systems with interaction [16, 17, 18, 19].

Consider now the general problem of two interacting electrons in a pure state. It is clear that in some circumstances this system reduces approximately to an equivalent system of two interacting spins, for which the above entanglement formula is appropriate. Furthermore, in the general case, entanglement between the spins of the fermions relates to measurements of spin irrespective of their orbital motion. We consider therefore spin-entanglement for a general class of two-electron states on a lattice of the form

$$|\Psi\rangle = \sum_{i,j=1}^N [\psi_{ij}^{\uparrow\downarrow} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \frac{1}{2}(\psi_{ij}^{\uparrow\uparrow} c_{i\uparrow}^\dagger c_{j\uparrow}^\dagger + \psi_{ij}^{\downarrow\downarrow} c_{i\downarrow}^\dagger c_{j\downarrow}^\dagger)] |0\rangle, \quad (2)$$

where c_{is}^\dagger creates an electron with spin s on site i and N is the total number of sites. The system in question could be, for example, a tight-binding lattice containing two valence electrons occupying non-degenerate atomic orbitals, or two electrons in the conduction band of a semiconductor, for which the sites represent finite-difference grid points. In either case, the interaction between the electrons is included together with any externally applied potential.

The two electrons are in separate regions of space (measurement domains) $[A]$ and $[B]$ as illustrated in Fig. 1(a). Entanglement might be produced, for example, when two initially unentangled electrons in wave packets approach each other and interact [Fig. 1(b)] and then again become well separated into distinct regions $[A]$ and $[B]$ [Fig. 1(c)]. Here one should realise that in real measurements of entanglement, indistinguishable electrons would be detected and the formalism relevant to distinguishable spins is not directly applicable. Nevertheless, complete information regarding the spin properties of such a fermionic system is contained in spin correlation

functions for the two domains. The spin-measuring apparatus would measure spin correlation functions for two domains $[A]$ and $[B]$ rather than for two distinguishable spins A and B .

Concurrence as a measure of entanglement for two electrons is related to the eigenvalues of the non-Hermitian matrix $\rho\tilde{\rho}$, where ρ is reduced density matrix given in terms of the electron spin correlations corresponding to the domains, and $\tilde{\rho}$ is the time-reversed density matrix as in Ref. 4. In general the eigenvalues of $\rho\tilde{\rho}$ can be determined only numerically and a closed form for concurrence can not be obtained, unless the system exhibits additional symmetries. Possible symmetries are conveniently studied through spin-spin correlation functions. We express spin operators for domains $[A]$ and $[B]$ with fermionic operators as the sum of operators for sites i within the domain $[A]$ (or $[B]$), i.e., $S_A^\lambda = \frac{1}{2} \sum_{i \in [A]} \sum_{ss'} c_{is}^\dagger \sigma_{ss'}^\lambda c_{is'}$, where σ^λ are Pauli matrices. For axially symmetric problems [20], where $\langle \Psi | S_{A(B)}^{\lambda=x,y} | \Psi \rangle = 0$ and $\langle \Psi | S_{A(B)}^z S_{B(A)}^{\lambda=x,y} | \Psi \rangle = 0$, concurrence may be written as

$$\begin{aligned} C &= \max(0, C_{\uparrow\downarrow}, C_{\parallel}), \\ C_{\uparrow\downarrow} &= 2|\langle S_A^+ S_B^- \rangle| - 2\sqrt{\langle P_A^\uparrow P_B^\uparrow \rangle \langle P_A^\downarrow P_B^\downarrow \rangle}, \\ C_{\parallel} &= 2|\langle S_A^+ S_B^+ \rangle| - 2\sqrt{\langle P_A^\uparrow P_B^\downarrow \rangle \langle P_A^\downarrow P_B^\uparrow \rangle}, \end{aligned} \quad (3)$$

where $S_{A(B)}^\pm = (S_{A(B)}^\mp)^\dagger = \sum_{i \in A(B)} c_{i\uparrow}^\dagger c_{i\downarrow}$ are spin raising operators for domains $[A]$ or $[B]$ and $P_{A(B)}^s = \sum_{i \in A(B)} n_{is}(1 - n_{i,-s})$, with $n_{is} = c_{is}^\dagger c_{is}$, are spin- s projectors operating in domains $[A]$ (or $[B]$). Fermionic expectation values required in Eq. (3) are then given in terms of the amplitudes in the normalised $|\Psi\rangle$ as

$$\begin{aligned} \langle S_A^+ S_B^- \rangle &= \sum_{[ij]} \psi_{ij}^{\uparrow\downarrow*} \psi_{ji}^{\uparrow\downarrow}, \\ \langle S_A^+ S_B^+ \rangle &= \sum_{[ij]} \psi_{ij}^{\uparrow\uparrow*} \psi_{ij}^{\uparrow\uparrow}, \\ \langle P_A^\uparrow P_B^\downarrow \rangle &= \sum_{[ij]} |\psi_{ij}^{\uparrow\downarrow}|^2, \\ \langle P_A^\downarrow P_B^\uparrow \rangle &= \sum_{[ij]} |\psi_{ji}^{\uparrow\downarrow}|^2, \end{aligned} \quad (4)$$

where the summation in Eq. (4) extends over all pairs $[ij]$ such that $i \in [A]$ and $j \in [B]$. In analogy to the Bell basis [1] one can introduce $\varphi_{ij}^\pm = (\psi_{ij}^{\uparrow\downarrow} \pm \psi_{ji}^{\uparrow\downarrow})/\sqrt{2}$ and $\chi_{ij}^\pm = (\psi_{ij}^{\uparrow\uparrow} \pm \psi_{ij}^{\downarrow\downarrow})/\sqrt{2}$. φ_{ij}^\pm , e.g., are the amplitudes for creating two electrons in a delocalised singlet or triplet state with zero total spin projection. It then follows from Eqs. (3 and 4) that the electrons are completely entangled, when either (i) $\varphi_{ij}^- = i c \varphi_{ij}^+$, $\chi_{ij}^\pm = 0$, or (ii) $\chi_{ij}^- = i c \chi_{ij}^+$, $\varphi_{ij}^\pm = 0$, where c is a real constant. In the general case (i.e., without spin symmetries) $C = 1$ if

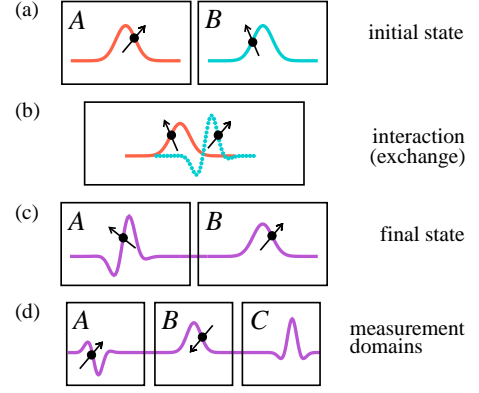


Figure 1: (Color online) (a) In each of the domains $[A]$ and $[B]$ the probability of finding one electron is equal, $n_A = n_B = 1$. (b) Interacting electrons with possible exchange, (c) separated electrons, and (d) several measurement domains, $n_A + n_C = n_B = 1$.

$|\psi\rangle$ is a linear combination of AB -entangled pair states, $|\psi\rangle = \sum_{[ij]} \psi_{ij} \sum_{\beta=1}^4 b_\beta |ij, \beta\rangle$, where $|ij, \beta\rangle$ are the Bell states [21] corresponding to pairs $[ij]$ and b_β are constants with $|\sum_{\beta=1}^4 b_\beta^2| = \sum_{[ij]} |\psi_{ij}|^2 = 1$.

When $|\Psi\rangle$ is an eigenstate of the total spin projection S_{tot}^z , Eqs. (3) and (4) simplify further. In particular, $C = 0$ if $S_{\text{tot}}^z = \pm 1$, while for $S_{\text{tot}}^z = 0$ the concurrence is given solely with the overlap between $|\Psi\rangle$ and the particular AB -spin-flipped state $|\tilde{\Psi}\rangle = S_A^+ S_B^- |\Psi\rangle$, Eq. (4), or as,

$$C = C_{\uparrow\downarrow} = \left| \sum_{[ij]} [(\varphi_{ij}^+)^2 - (\varphi_{ij}^-)^2] \right|. \quad (5)$$

If probabilities for singlet and triplet are equal, the concurrence formula reduces to $C = 2|\text{Im} \sum_{[ij]} (\varphi_{ij}^+)^* \varphi_{ij}^-|$ and if $\varphi_{ij}^+ = \varphi_{ij}^- e^{i\delta}$, to $C = |\sin \delta|$. If the state $|\Psi\rangle$ corresponds to the system in continuum space, $i \rightarrow \mathbf{r} = (x, y, z)$, the only change is that summations are replaced by integrations of $\varphi^\pm = \langle \mathbf{r}_1, \mathbf{r}_2; S_{\text{tot}} | \Psi \rangle$ over the corresponding measurement domains, e.g., $C = |\int_{[A]} \int_{[B]} [(\varphi^+)^2 - (\varphi^-)^2] d^3 \mathbf{r}_1 d^3 \mathbf{r}_2|$.

In order to illustrate how these concurrence formulae can be applied in practice, as the first example we consider two interacting electrons on a one-dimensional lattice with $N \rightarrow \infty$ and with the hamiltonian, $H_0 = -t_0 \sum_{is} (c_{is}^\dagger c_{i+1,s} + h.c.) + \sum_{ijss'} U_{ij} n_{is} n_{js'}$.

To be specific, let one electron with spin \uparrow be confined initially to the region A ($i \sim -L$) and the other electron in region B ($i \sim L$) with opposite spin, Fig. 2(a). The simplest initial state is two wave packets with vanishing momentum uncertainty $\Delta k \rightarrow 0$, the left with momentum $k > 0$ and the right with $q < 0$. After collision the electrons move apart with probability amplitude t_{kq} for non-spin-flip scattering and spin-flip amplitude r_{kq} . More general initial wave packets are defined with mo-

momentum amplitudes ϕ_k and $\bar{\phi}_q$ for spin \uparrow and \downarrow , respectively. Concurrence Eq. (5) after the collision is then expressed as

$$C = 2 \left| \iint t_{kq}^* r_{kq} |\phi_k|^2 |\bar{\phi}_q|^2 dk dq \right|, \quad (6)$$

which simplifies to $C \sim 2|t_{kq}r_{kq}|$ for sharp momentum resolution wave packets, with $k = -q = k_0$. Note that $C = 1$ when spin-flip and non-spin-flip amplitudes coincide in accord with recent analysis of flying and static qubits entanglement [22, 23, 24] or of scattering of distinguishable particles [14].

Consider the prototype finite range interaction, $U_{ij} = \frac{1}{2}U \sum_{m=0}^M \delta_{|i-j|,m}$. The Hubbard model ($M = 0$) can be solved analytically in one-dimension [25] and the amplitudes are $t_{kq} = 1 + r_{kq} = (\sin k - \sin q)/[(\sin k - \sin q) + iU/(2t_0)]$. In Fig. 2(a) concurrence is presented for wave packets with well defined momentum k_0 for $U = t_0$, together with a longer range interaction case, $M = 3$, for sharp momentum (full line) and for a Gaussian initial amplitude $\bar{\phi}_k = \phi_{-k}$ with $\Delta k = \pi/10$ (dashed line). An interesting observation here is substantial reduction of concurrence due to the coherent averaging in Eq. (6). Additionally, electrons will be completely entangled at some kinetic energy comparable with the repulsion, $U \sim 2t_0(1 - \cos k_0)$, where spin-flip and non-spin-flip amplitudes coincide.

The concurrence formula Eq. (5) is derived for electronic states when double occupancy is negligible, i.e., $\psi_{ii}^{\uparrow\downarrow} \rightarrow 0$, which in our case is strictly fulfilled only asymptotically when the electrons are far apart. However, Eq. (5) can be evaluated at any time t and the resulting $C(t)$ can serve as a measure of entanglement during the transition from initial to final state. In Fig. 2(b) we present the time dependence of $C(t)$ for some typical k_0 , with $M = 5$ and $U = 2t_0$. Oscillation with t can be interpreted as response to the finite time duration of electron-electron interaction and the model can be approximately mapped onto an effective Heisenberg model, for which concurrence oscillates as $C(t) = |\sin J_{\text{eff}} t|$, where J_{eff} is the effective antiferromagnetic coupling between the electrons.

Another important example is the concurrence of flying-static qubits in experiments in which the system is prepared with a static electron bound in some confining potential (region [B]) and a flying electron injected in some distant region [A] [22, 23]. Contrary to the previous case with translation symmetry, after the collision there are nonvanishing amplitudes for transmission (into region [C]) and reflection (back into region [A]), as shown in Fig. 1(d).

Let the initial state be prepared as $\varphi_{ij}^{\pm} = (b_i g_j \pm g_i b_j)/\sqrt{2}$, where b_i is the orbital state of the bound electron with spin \downarrow centered around $i \sim 0$. Similarly, $g_j \propto \int \phi_k e^{i[k(j+L) - \omega_k t]} dk$ is the initial orbital

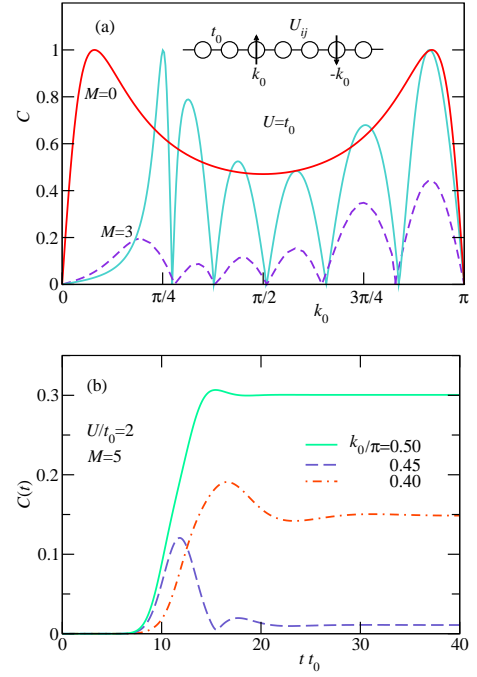


Figure 2: (Color online) (a) C for: (i) the Hubbard model ($M = 0$) for $U = t_0$ and $\Delta k = 0$; (ii) $M = 3$: for $\Delta k = 0$ (full line) and $\Delta k = \pi/10$ (dashed). (b) $C(t)$ for Gaussian packets with various k_0 and $M = 5$, $U = 2t_0$ and $\Delta k = \pi/20$. At $t = 0$ the separation between the packets is $2L = 10/\Delta k$.

state of the propagating electron with spin \uparrow , centered around $i \sim -L$ and moving in the positive i -direction with momentum amplitude ϕ_k peaked at $k \sim k_0$, and with momentum uncertainty $\Delta k \rightarrow 0$. Here we consider elastic scattering with amplitudes after the collision, $\varphi_{ij}^{\pm} = r_{\pm}(b_i a_j \pm a_i b_j) + t_{\pm}(b_i c_j \pm c_i b_j)$, where $r_{\pm}(k_0)$ and $t_{\pm}(k_0)$ are singlet (triplet) reflection and transmission amplitudes and a_j, c_j are normalised wave packets with mean momentum $-k_0$ and k_0 , respectively.

Two basic experimental setups are possible when electrons are detected in different measurement domains, $[AB]$ or $[BC]$. Concurrence corresponding to reflected qubits is then

$$C_{AB} = \frac{2|\langle S_A^+ S_B^- \rangle|}{n_A n_B} \sim \frac{|r_+^2(k_0) - r_-^2(k_0)|}{|r_+(k_0)|^2 + |r_-(k_0)|^2}, \quad (7)$$

where $n_A = \langle \sum_{s,i \in [A]} n_{is} \rangle$, $n_B = 1$ [26]. Concurrence for transmitted qubits, C_{BC} , is given by an analogous expression with $A \rightarrow C$, and consequently with r_{\pm} replaced with t_{\pm} . If the measuring apparatus captures both, reflected and transmitted electrons ($i \in [A] \cup [C]$, $j \in [B]$), concurrence is given by $C_{AC,B} = |(r_+ - r_-)^*(r_+ + r_-) + (t_+ - t_-)(t_+ + t_-)^*|$ and no additional renormalisation is required. Eq. (7) also follows directly from Eq. (1) if appropriately applied to scattering states [22, 23]. However, for finite Δk , C_{AB} (and correspondingly C_{BC} or

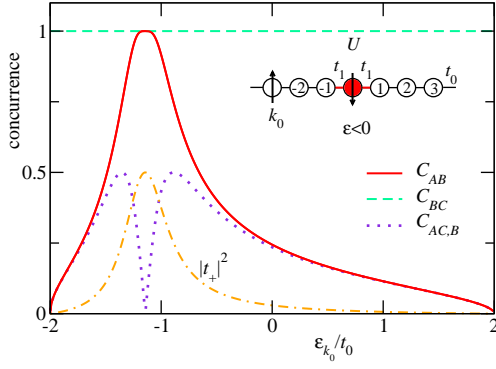


Figure 3: (Color online) Concurrence corresponding to various domains for infinite- U Anderson model with $\epsilon + U = -t_0$, $t_1 = t_0/4$ and $\Delta k \rightarrow 0$. Dashed dotted line represents the singlet transmission probability $|t_+|^2$.

$C_{AC,B}$) has to be rederived from Eq. (5),

$$C_{AB} = \frac{|\int [r_+^2(k) - r_-^2(k)] |\phi_k|^2 dk|}{\int [|r_+(k)|^2 + |r_-(k)|^2] |\phi_k|^2 dk}. \quad (8)$$

In order to demonstrate the basic properties of C_{AB} and C_{BC} we consider here the Anderson model, $H = H_0 + \sum_s [\epsilon n_{0s} - (t_1 - t_0)(c_{-1s}^\dagger c_{0s} + c_{0s}^\dagger c_{1s} + h.c.)]$, where H_0 is the Hubbard hamiltonian in which $U = 0$ except for the impurity site, $\epsilon < 0$ is the impurity energy level, and t_1 is the hopping matrix element connecting the impurity site $i = 0$ with left and right leads.

In the large- U regime, $U, -\epsilon \gg t_0$, the static electron is strongly localised, $b_i \sim \delta_{i0}$. Electrons in the triplet channel are reflected, $r_- = -\frac{1}{\sqrt{2}}$, $t_- = 0$, while singlet scattering amplitudes exhibit 'charge transfer' resonance: $t_+ = \frac{1}{\sqrt{2}} + r_+ = \frac{2}{\sqrt{2}} \Gamma_k / (\epsilon_k - \omega_0 + i\Gamma_k)$ with $\epsilon_k = -2t_0 \cos k$, $\omega_0 = (\epsilon + U)/(1 - 2t_1^2/t_0^2)$ and $\Gamma_k = 2t_1^2(4t_0^2 - \omega_k^2)^{1/2}/(t_0^2 - 2t_1^2)$ [27]. 'Transmitted' concurrence is due to the missing triplet amplitude, trivially, $C_{BC} \equiv 1$. Reflected electrons are completely entangled at the singlet resonance energy but 'total' concurrence $C_{AC,B} = 0$ there, as shown in Fig. (3).

The main result of this work is the closed form formulae of Wootters entanglement measure defined for two delocalised electrons. The proposed approach enables simple analysis of entanglement for a variety of realistic problems, from scattering of flying and static qubits represented as wave packets with finite energy resolution, to time evolution of static qubits due to electron-electron interaction or due to externally applied fields. Further application to systems described with mixed states or with more than two electrons is possible, however, an appropriate definition of entanglement valid also for systems with non-negligible doubly occupancy, remains open.

We thank L. Amico, C.W.J. Beenakker, G. Falci, A. Fubini, and T.P. Spiller for helpful discussions. AR and IS acknowledge support from the Slovenian Research

Agency under contract PI-0044, and JHJ support from the UK Ministry of Defence.

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